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by

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We adopt a continuous model to estimate the Grothendieck constants. An analytical formula to compute the lower bounds of Grothendieck constants has been explicitly derived for arbitrary orders, which improves previous bounds. Moreover, our lower bound of the Grothendieck constant of order three gives a refined bound of the threshold value for the nonlocality of the two-qubit Werner states.

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I. INTRODUCTION

Quantum mechanics exhibits the nonlocality of the nature in essence. The impossibility of reproducing all correlations observed in composite quantum systems using models à la Einstein-Podolsky-Rosen (EPR) [1] was proven in 1964 by Bell [2]. A quantum state is said to admit a local hidden variable (LHV) model if all the measurement outcomes can be modeled as a classical random distribution over a probability space. Consider a bipartite state ρ in $\mathcal{H}_{\mathtt{A}}\otimes\mathcal{H}_{\mathtt{B}}$ with subsystems $\mathtt{A}$ and $\mathtt{B}$. If Alice performs a measurement A on the subsystem $\mathtt{A}$ with an outcome a_i and, at space-like separation, Bob performs a measurement B on the subsystem $\mathtt{B}$ with an outcome b_j, then an LHV model supposes that the joint probability of getting a_i and b_j satisfies

$$\Pr(a_i, b_j|A, B, \rho) = \int_\Omega \Pr(a_i|A, \lambda)\Pr(b_j|B, \lambda)\, d\omega^\rho(\lambda),$$

where $d\omega^\rho(\lambda)$ is some distribution over a space Ω of hidden variable λ. A quantum state is called *local* if it admits an LHV model, and *nonlocal* otherwise.

In his seminal work, Bell showed that all quantum states admitting LHV models satisfy the so-called Bell inequalities [2]. That is, a state admits no LHV models if it violates some Bell inequalities. It is known that every pure entangled bipartite or multipartite state violates a generalized Bell inequality [3, 4]. Namely, for pure states the entanglement and the non-locality coincide. However for mixed states, the situation is more complicated. There are no general methods to judge whether a mixed state admits an LHV model or not, i.e. to find all Bell inequalities is computationally hard [5, 6]. Even for the most concerning two-qubit Werner states, the precise threshold value of nonlocality is still unknown.

As the "fundamental theorem in the metric theory of tensor products", the Grothendieck's theorem [7] had a major impact on Banach space theory. The constants related to the Grothendieck's theorem are nowadays called Grothendieck constants [8]. It turns out that the Grothendieck constants are connected to the Bell inequalities, observed by Tsirelson [9]. Of particular interest, Acin-Gisin-Toner [10] demonstrated that the threshold value for the non-locality of the Werner states for projective measurements is given explicitly by the Grothendieck constant of order three, $K(3)$, see Section II for the definition. This reduces the problem of the nonlocality of Werner states to the computation of the exact value of $K(3)$. However, it is formidably difficult to compute the Grothendieck constants except for the case of order two. Generally, what one can do is to estimate the lower and upper bounds of the Grothendieck constants.

In this paper, by generalizing the Bell operator with 465 measurement settings on each side in [11] to a continuous model with infinitely many measurement settings, we present an analytical formula in estimating the lower bounds of the Grothendieck constants. This formula is valid for Grothendieck constants of arbitrary order and improves many previously obtained bounds. From our lower bound of $K(3)$, we derive a bound of the threshold value for the nonlocality of the two-qubit Werner states, which gives the best knowledge about such nonlocality up to date.

II. LOWER BOUND OF GROTHENDIECK CONSTANT FOR ARBITRARY ORDER d

Let $\mathcal{M}_m(\mathbb{R})$ be the set of $m\times m$ real matrices and S^{d-1} the unit sphere in $\mathbb{R}^d$, $m, d \in \mathbb{N}$. Given $M \in \mathcal{M}_m(\mathbb{R})$, we define

$$C(M) = \sup \left| \sum_{i,j=1}^m M_{ij}\, a_i b_j \right|, \tag{1}$$

where the supremum is taken over all possible assignment $a_i, b_j \in \{1, -1\}$, $1 \le i, j \le m$. Replacing a_i, b_j by d-dimensional unit vectors, we define

$$Q(M) = \sup_{\mathbf{a_i},\mathbf{b_j}\in S^{d-1}} \left| \sum_{i,j=1}^m M_{ij}\, \mathbf{a_i}\cdot\mathbf{b_j} \right|,$$

where the supremum is taken over all d-dimensional unit vectors $\mathbf{a_i}$ and $\mathbf{b_j}$ and $\mathbf{a_i}\cdot\mathbf{b_j}$ denotes their scalar product. The Grothendieck constant of order d is defined by

$$K(d) = \sup_{m\geq 1} \sup_{\substack{M\in\mathcal{M}_m(\mathbb{R})\\ M\neq 0}} \frac{Q(M)}{C(M)}. \quad (2)$$

The value of $C(M)$ depends only on the choice of the matrix M. Besides M, $Q(M)$ also depends on the dimension d of Euclidean space $\mathbb{R}^d$ where we choose unit vectors $\mathbf{a_i}$ and $\mathbf{b_j}$. It is a great challenge to evaluate the Grothendieck constant $K(d)$ for general d. Till now the only exactly known result of $K(d)$ is for $d = 2$, $K(2) = \sqrt{2}$ [12]. For $d \geq 3$, there are some lower bounds of $K(d)$: For instance, Briët-Buhrman-Toner [13] obtained a lower bound of $K(d)$ for general d,

$$K(d) \geq \frac{\pi}{d}\left(\frac{\Gamma(\frac{d+1}{2})}{\Gamma(\frac{d}{2})}\right)^2.$$

In this section, we propose a continuous model to compute the lower bounds of the Grothendieck constant for arbitrary d. Our results improve some known lower bounds. In particular, the lower bound of $K(3)$ we obtained is the best up to date, which improves the result on non-locality of the Werner states.

For any $n \in \mathbb{N}$, let $m = n + n(n-1)/2$. We choose the following special $M \in M_m(\mathbb{R})$ such that [11]

$$C(M) = \sup\left|\sum_{i,j=1}^{n} a_i b_j + \sum_{i<j}[\alpha_{ij}(b_i - b_j) + \beta_{ij}(a_i - a_j)]\right|,$$

where the supremum is taken over $a_i, \alpha_{ij} \in \{1, -1\}$ and $b_j, \beta_{ij} \in \{1, -1\}$ ($\{a_i, \alpha_{ij}\}$ stands for $\{a_i\}_{i=1}^m$ in the definition (1), similarly $\{b_i, \beta_{ij}\}$ for $\{b_j\}_{j=1}^m$). Hence by choosing $\alpha_{ij} = \mathrm{sign}(b_i - b_j)$ and $\beta_{ij} = \mathrm{sign}(a_i - a_j)$, one has

$$C(M) = \sup\left|\sum_{i,j=1}^{n} a_i b_j + \sum_{i<j}(|b_i - b_j| + |a_i - a_j|)\right| = n^2.$$

Correspondingly, for given M, to get a better bound of $Q(M)$ one needs to suitably choose the vectors $\mathbf{a_i}$ and $\mathbf{b_j}$. By setting vectors $\alpha_{\mathbf{ij}}$ ($\beta_{\mathbf{ij}}$ resp.) parallel to $\mathbf{b_i} - \mathbf{b_j}$ ($\mathbf{a_i} - \mathbf{a_j}$ resp.) and $\mathbf{a_i} = \mathbf{b_i}$, $1 \leq i \leq n$, one obtains

$$Q(M) = \sup_{\mathbf{a_i}\in S^{d-1}}\left(|\sum_i \mathbf{a_i}|^2 + 2\sum_{i<j}|\mathbf{a_i} - \mathbf{a_j}|\right). \quad (3)$$

Therefore

$$K(d) \geq \sup_{\mathbf{a_i}\in S^{d-1}}\left(\left|\frac{1}{n}\sum_i \mathbf{a_i}\right|^2 + \frac{1}{n^2}\sum_{i\neq j}|\mathbf{a_i} - \mathbf{a_j}|\right), \quad (4)$$

where the supremum is taken over $(\mathbf{a_1}, \cdots, \mathbf{a_n}) \in (S^{d-1})^n$ for any $n \geq 1$.

Using this discrete version of optimization problem, Vértesi [11] runs a numerical simulation to obtain the lower bounds of $K(d)$, $3 \leq d \leq 5$. Since the complexity of the computation grows exponentially, the computation of the lower bounds becomes impossible for large d. Instead of this, we propose a continuous model to reformulate this problem. Let $P(S^{d-1})$ denote the space of probability measures on S^{d-1}. Then we have

Theorem II.1. *For $d \geq 1$,*

$$K(d) \ \geq\ \sup_{\mu\in P(S^{d-1})}\Big(\big|\int_{S^{d-1}} \mathbf{x}\, d\mu(\mathbf{x})\big|^2 + \int_{S^{d-1}\times S^{d-1}} |\mathbf{x} - \mathbf{y}|\, d\mu(\mathbf{x})d\mu(\mathbf{y})\Big). \quad (5)$$

Proof. From the discrete version (4), the assertion (5) holds for rational convex combination of delta measures, i.e. $\mu = \sum_{i=1}^N \lambda_i \delta_{\mathbf{a_i}}$ with $\lambda_i \in \mathbb{Q}_+$, $\sum_{i=1}^N \lambda_i = 1$ and $\mathbf{a_i} \in S^{d-1}$. Since any probability measure $\mu \in P(S^{d-1})$ can be approximated by convex combination of delta measures (in the weak topology) and $|\mathbf{x}|, |\mathbf{x} - \mathbf{y}|$ are continuous functions, the theorem follows from the definition of weak convergence of measures. □

Hence, to derive an effective lower bound of $K(d)$ it suffices to choose some good measures for this optimization problem. It seems that the problem becomes more complicated since the finite dimensional optimization problem has been transformed to an infinite dimensional problem on the space of measures. However, this is in fact an advantage which allows one to choose nice absolutely continuous measures on a sphere to get explicit lower bounds of the Grothendieck constants.

Let $(\phi_1, \phi_2, \cdots, \phi_{d-1})$ be the spherical coordinates of $S^{d-1} \subset \mathbb{R}^d$ such that

$$\begin{cases} x_1 = \sin\phi_1 \sin\phi_2 \cdots \sin(\phi_{d-1}), \\ x_2 = \sin\phi_1 \sin\phi_2 \cdots \cos(\phi_{d-1}), \\ \cdots \\ x_{d-1} = \sin\phi_1 \cos\phi_2, \\ x_d = \cos\phi_1, \end{cases}$$

where $\phi_i \in [0, \pi]$ for $1 \leq i \leq d-2$ and $\phi_{d-1} \in [0, 2\pi)$. We denote by $d\mu = \sin^{d-2}\phi_1 \sin^{d-3}\phi_2 \cdots \sin\phi_{d-2}\, d\phi_1 d\phi_2 \cdots d\phi_{d-1}$ the spherical (volume) measure of S^{d-1}. For simplicity, we also denote by $\mathbf{x} = (\mathbf{x}', x_d)$, $\mathbf{x}' \in \mathbb{R}^{d-1}$, the Cartesian coordinates of $\mathbf{x} \in S^{d-1}$, by $P_d(\mathbf{x}) = x_d$ the projection to the d-th coordinate, and by $\phi_1(\mathbf{x})$ the first spherical coordinate of $\mathbf{x}$. For any $0 \leq a \leq b \leq \frac{\pi}{2}$, we denote

$$\Omega_a^b = \{\mathbf{x} \in S^{d-1} : a \leq \phi_1(\mathbf{x}) \leq b\},$$

which is contained in the upper hemisphere $S^{d-1} \cap \{x_d \geq 0\}$. To obtain the lower bounds of $K(d)$, we will choose the uniform probability measure on Ω_a^b, i.e. $\mu_{a,b} = \frac{1}{\mathrm{vol}\,\Omega_a^b}\mathrm{vol}|_{\Omega_a^b}$. The variables a, b are introduced to refine (i.e. maximize in some sense) the lower bound of $K(d)$, since we have no priori knowledge of the optimal measure which attains the maximum on the right hand side of (5).

Then second term of the right hand side of (5) corresponds to

$$\int_{\Omega_a^b\times\Omega_a^b} |\mathbf{x}-\mathbf{y}|d\mu_{a,b}(\mathbf{x})d\mu_{a,b}(\mathbf{y}) = \frac{1}{\mathrm{vol}(\Omega_a^b)^2}\int_{\Omega_a^b\times\Omega_a^b} |\mathbf{x}-\mathbf{y}|d\mu(\mathbf{x})d\mu(\mathbf{y}),$$

which involves a $2(d-1)$-multiple integration. This is the obstruction for the numerical computation of the lower bounds for large d. Nevertheless, the computation can be considerably simplified by the symmetry of the sphere.

Lemma 1. *For any* $\mathbf{x}, \tilde{\mathbf{x}} \in S^{d-1}$ *satisfying* $\phi_1(\mathbf{x}) = \phi_1(\tilde{\mathbf{x}})$, *we have*

$$\int_{\Omega_a^b} |\mathbf{x}-\mathbf{y}|d\mu(\mathbf{y}) = \int_{\Omega_a^b} |\tilde{\mathbf{x}}-\mathbf{y}|d\mu(\mathbf{y}). \tag{6}$$

Proof. For given $\mathbf{x}$ and $\tilde{\mathbf{x}}$ with $P_d(\mathbf{x}) = P_d(\tilde{\mathbf{x}})$, there is an isometry of S^{d-1}, $A \in SO(d)$, such that $A(\mathbf{x}) = \tilde{\mathbf{x}}$ and $A(\Omega_a^b) = \Omega_a^b$. This can be seen as follows: Without loss of generality, one may write $\mathbf{x} = (\mathbf{x}', c)$ and $\tilde{\mathbf{x}} = (\tilde{\mathbf{x}}', c)$ where $c = P_d(\mathbf{x})$. Since $\mathbf{x}', \tilde{\mathbf{x}}' \in \sqrt{1-c^2}\, S^{d-2}$, there is a $B \in SO(d-1)$ such that $B\mathbf{x}' = \tilde{\mathbf{x}}'$. Hence one can take

$$A = \begin{pmatrix} B & 0 \\ 0 & 1 \end{pmatrix}.$$

Since $SO(d)$ acts isometrically on S^{d-1}, the equation (6) follows. □

By the Lemma, for given $\mathbf{x} \in \Omega_a^b$ the integral over $\mathbf{y}$ only depends on $\phi_1(\mathbf{x})$. Without loss of generality, we may choose $\mathbf{x} = (0, 0, \cdots, \sin\phi_1, \cos\phi_1)$, i.e. its spherical coordinate is $(\phi_1, 0, \cdots, 0)$. Then for any $\mathbf{y}$ whose spherical coordinate reads $(\psi_1, \psi_2, \cdots, \psi_{d-1})$, one has

$$|\mathbf{x}-\mathbf{y}| = \sqrt{2 - 2\sin\phi_1\sin\psi_1\cos\psi_2 - 2\cos\phi_1\cos\psi_1}. \tag{7}$$

Therefore we obtain

$$\int_{\Omega_a^b\times\Omega_a^b} |\mathbf{x}-\mathbf{y}|d\mu(\mathbf{x})d\mu(\mathbf{y}) = \mathrm{vol}(S^{2-3})\mathrm{vol}(S^{d-3})\int_a^b\int_a^b\int_0^\pi f(\phi_1,\psi_1,\psi_2)d\phi_1 d\psi_1 d\psi_2$$

for $d \geq 3$, where

$$f(\phi_1,\psi_1,\psi_2) = |\mathbf{x}-\mathbf{y}|\sin^{d-2}\phi_1\sin^{d-2}\psi_1\sin^{d-3}\psi_2, \tag{8}$$

with $|\mathbf{x}-\mathbf{y}|$ given by (7). Combining above results, we have the following theorem:

Theorem II.2. *The Grothendieck constant* $K(d)$, $d \geq 3$, *satisfies*

$$K(d) \geq \frac{1}{\left(\int_a^b \sin^{d-2}\phi_1 d\phi_1\right)^2}\left[\left(\frac{\sin^{d-1}\phi_1}{d-1}\Bigg|_a^b\right)^2 + \frac{\mathrm{vol}(S^{d-3})}{\mathrm{vol}(S^{d-2})}\int_a^b\int_a^b\int_0^\pi f(\phi_1,\psi_1,\psi_2)d\phi_1 d\psi_1 d\psi_2\right], \tag{9}$$

where $f(\phi_1,\psi_1,\psi_2)$ *is given by* (8).

By reducing a $2(d-1)$-multiple integration to a triple integration for any $d \geq 3$, we have obtained a lower bound of the Grothendieck constants which can be easily calculated via numerical methods. By varying a, b in the domain $\{(a,b) : 0 \leq a < b \leq \frac{\pi}{2}\}$, one may get a refined lower bound of $K(d)$ by maximizing the right hand of (9) for these a, b. For instance, by taking $a = 0$, $b = 1.04819755$, one gets $K(3) \geq 1.41758$. Taking $a = 0.742832$, $b = 0.749115$, one gets $K(5) \geq 1.46112$. Some numerical results are listed in the following table:

	$K(d) \geq$		
d	Vértesi	Briët etc.	our result
3	1.41724	1.33333	1.41758
4	1.44521	1.38791	1.44566
5	1.46007	1.42222	1.46112
6		1.44574	1.47017
7		1.46286	1.47583
8		1.47586	1.47972

The first column collects the results of Vértesi [11] for the case $d = 3, 4, 5$. The second column contains the lower bounds of $K(d)$ proved by Briët-Buhrman-Toner [13]. From this table, one immediately figures out that our results improve the results of Vértesi [11] and Briët-Buhrman-Toner [13] for $d \leq 8$.

III. NON-LOCALITY OF TWO-QUBIT WERNER STATES

In 1989, Werner explicitly constructed LHV models for some entangled mixed bipartite states[14]. The two-qubit Werner state is given by

$$\rho_p^W = p\,|\psi^-\rangle\langle\psi^-| + (1-p)\mathbb{I}/4, \tag{10}$$

where in computational basis, $|\psi^-\rangle = (|01\rangle - |10\rangle)/\sqrt{2}$ and $0 \le p \le 1$. ρ_p^W is separable if and only if $p \le 1/3$ [14]. It admits an LHV model for all measurements for $p \le 5/12$ [15], and admits an LHV model for projective measurements for $p \le 0.6595$ [10].

Let A_i and B_i, $i = 1, 2, ..., m$, be dichotomic observables with respect to the two qubits, $A_i = \mathbf{a}_i \cdot \sigma$ and $B_i = \mathbf{b}_i \cdot \sigma$, with $\sigma = (\sigma_1, \sigma_2, \sigma_3)$ the Pauli matrices. $\mathbf{a}_i = (a_i^{(1)}, a_i^{(2)}, a_i^{(3)})$, $\mathbf{b}_i = (b_i^{(1)}, b_i^{(2)}, b_i^{(3)})$ are 3-dimensional real unit vectors. For any Bell operator,

$$B(M) = \sum_{i,j=1}^{m} M_{ij}\, A_i \otimes B_j,$$

where $M \in \mathcal{M}_m(\mathbb{R})$ as in (1), the mean value is given by

$$Tr(B(M)\rho_p^W) = p \sum_{i,j=1}^{m} M_{ij}\, \mathbf{a_i} \cdot \mathbf{b_j}.$$

Therefore the maximal violation of the corresponding Bell inequality is given by $p\,K(3)$ and ρ_p^W admits LHV models for projective measurements if and only if $p \le 1/K(3)$ [10]. Hence the nonlocality problem of the two-qubit Werner states is reduced to estimate the value of $K(3)$.

However, the precise value of $K(3)$ is still unknown. There are various attempts to derive the upper and lower bounds of the Grothendieck constants. For instance, Krivine [12] showed that $K(3) \le 1.5163$. The Clauser-Horne-Shimony-Holt (CHSH) inequality implies that $K(3) \ge \sqrt{2}$, [16]. Vértesi [11] constructed Bell inequalities involving 465 settings on each qubit ($\{A_i, B_i\}_{i=1}^m$, $m \ge 465$) to show that $K(3) \ge 1.417241$, i.e., ρ_p^W admits no LHV models for $p > 0.705596$. From Theorem II.2, we have shown that $K(3) \ge 1.41758$. Therefore ρ_p^W admit no LHV models for $p > 0.705428$. This provides the best known bound for the nonlocality of two-qubit Werner states, see Fig. 1: Acin-Gisin-Toner show that ρ_p^W admits LHV models for $p \le 0.66$. Vertesi shows that ρ_p^W admits no LHV models for $p > 0.705597$. We show that ρ_p^W admits no LHV models for $p > 0.705428$.

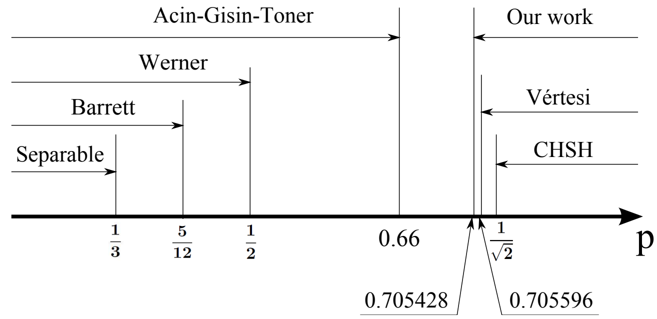

FIG. 1: Nonlocal properties of two-qubit Werner states.

IV. CONCLUSION AND DISCUSSIONS

We have presented an analytical formula to estimate the lower bounds of the Grothendieck constants for arbitrary order. It has been shown that our bounds improve the previously obtained bounds for $d = 3, ..., 8$. It is also straightforward to calculate the lower bounds for higher order d.

Moreover, our lower bound of $K(3)$ gives a bound of the best threshold value for the nonlocality of the two-qubit Werner states up to date. In fact, our new lower bounds of the Grothendieck constant of high orders can be also used to improve the knowledge about the nonlocality for higher dimensional quantum states such that the related mean values of Bell operators are determined by the Grothendieck constants [10].

The quantum discord [17, 18] has been introduced in characterizing information correlations between two subsystems, which is the minimal amount of mutual information that can not be learned by any measurements only on one of the subsystems. The quantum discord is zero for all classical-classically correlated states and greater than zero for all quantum-classically (classical-quantum) or quantum-quantum correlated states. The quantum entanglement [19–21] has been introduced to certify if the measurements on one subsystem of a bipartite or multipartite state would affect the measurement outcomes from other subsystems. The entanglement measure, e.g. entanglement of formation and concurrence, gets zero for separable states and greater than zero for all entangled states. These quantities such as quantum discord, entanglement of formation and concurrence are well defined, though formidably difficult to compute analytically in general. Nevertheless, so far one has no such elegant quantities to justify if a quantum entangled state admits local hidden variable models. For two-qubit Werner states, the Grothendieck constant $K(3)$ here plays the similar role of quantum discord and concurrence [22] in the sense that $p\,K(3)-1$ is zero if ρ_p^W admits LHV models and greater than zero if not. It would be also interesting to find such quantities for general states.

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